



Spin-orbit coupling implementation in Abinit

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- Theoretical framework
- Abinit v3 modifications
- Running Abinit with spin-orbit coupling
- An example : α -uranium





Motivations

✓ Rare earths and actinides

Spin-orbit coupling cannot be neglected

✓ Complex structures:

Structural parameters have to be relaxed

Forces and stresses must be implemented

✓ Abinit

Plane-waves +pseudopotential approach





Spin-orbit coupling – History

Abinit v3.0

- Total energy and forces with spin-orbit

Abinit v3.1

- Stresses with spin-orbit
- Optimizations

Abinit v3.2

- Response to atomic displacements with spin-orbit

Response to an electric field not yet available





Theoretical framework – Briefly

1

↳ Spin-orbit

$$H = H_0 + \frac{1}{2c^2 r} \frac{dV}{dr} \vec{L} \cdot \vec{S} + \dots$$

$$\psi(\vec{r}) = \frac{1}{r} \begin{cases} G(r) \cdot Y_J^M \\ F(r) \cdot Y_J^M \end{cases}$$

$\psi(r)$: 2 components spinor

↳ Dirac equation

$$\begin{cases} \frac{dF}{dr} - \left(\frac{\kappa}{r} \right) \cdot F + [\varepsilon - V(r)] \cdot \alpha \cdot G = 0 \\ \frac{dG}{dr} + \left(\frac{\kappa}{r} \right) \cdot G + \left[\frac{2}{\alpha^2} + \varepsilon - V(r) \right] \cdot \alpha \cdot F = 0 \end{cases}$$

$$\begin{aligned} \alpha &= \frac{1}{c} \\ \begin{cases} \kappa = l & J = l - \frac{1}{2} \\ \kappa = -(l+1) & J = l + \frac{1}{2} \end{cases} \end{aligned}$$

↳ Mixing F and G

$$\frac{d^2 G}{dr^2} - \frac{\kappa \cdot (\kappa + 1)}{r^2} \cdot G + 2(\varepsilon_\kappa - V) \cdot G = 0$$

$$\alpha^2 \ll 1$$



Theoretical framework

- ↪ Pseudopotential treatment of G
For each channel $l+1/2$ and $l-1/2$

$$V^{PS} = \sum_{l,m} \left| \Phi_{l+\frac{1}{2}} \right\rangle \left\langle \Phi_{l+\frac{1}{2}} \right| + \sum_{m \text{ omitted}} \dots V_{l-\frac{1}{2}} \dots$$

$$\Phi_M^J = l.c. \begin{pmatrix} Y_m^l \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ Y_m^l \end{pmatrix} \begin{pmatrix} Y_{m\pm 1}^l \\ 0 \end{pmatrix} \begin{pmatrix} 0 \\ Y_{m\pm 1}^l \end{pmatrix}$$

- ↪ Kleinman-Bylander separation (adding/substracting V_L)

$$V^{PS} = V_L + \sum_{l,m} \frac{\left| \left(V_{l+\frac{1}{2}} - V_L \right) \Phi_{l+\frac{1}{2}} \right\rangle \left\langle \left(V_{l+\frac{1}{2}} - V_L \right) \Phi_{l+\frac{1}{2}} \right|}{\left\langle \Phi_{l+\frac{1}{2}} \left| \left(V_{l+\frac{1}{2}} - V_L \right) \Phi_{l+\frac{1}{2}} \right\rangle \right\rangle} + \sum_{l-\frac{1}{2}} \dots V_{l-\frac{1}{2}} \dots$$

...

$$V^{PS} = V_L + \sum_{l,m} \left| v_{l+\frac{1}{2}} \Phi_{l+\frac{1}{2}} \right\rangle \left\langle \Phi_{l+\frac{1}{2}} v_{l+\frac{1}{2}} \right| + \sum_{l-\frac{1}{2}} \dots v_{l-\frac{1}{2}} \dots$$

Theoretical framework

↳ v_l^{ion}, v_l^{so} adequate linear combination of $v_{l+1/2}$ and $v_{l-1/2} \dots$

$$V = V_L + v_{NL}^{ion-ion} + v_{NL}^{ion-so} + v_{NL}^{so-ion} + v_{NL}^{so-so}$$

$$v_{NL}^{ion-ion} = \sum_{l,m} \left| v_l^{ion} Y_l^m \right\rangle \left\langle Y_l^m v_l^{ion} \right|$$

$$v_{NL}^{ion-so} = \sum_{l,m} \left| v_l^{ion} Y_l^m \right\rangle \left\langle Y_l^m v_l^{so} \right| \vec{L} \cdot \vec{S}$$

$$v_{NL}^{so-so} = \sum_{l,m} \left| \vec{L} \cdot \vec{S} \right| v_l^{so} Y_l^m \left\langle Y_l^m v_l^{so} \right| \vec{L} \cdot \vec{S}$$

$$v_{NL}^{so-ion} = \sum_{l,m} \left| \vec{L} \cdot \vec{S} \right| v_l^{so} Y_l^m \left\langle Y_l^m v_l^{ion} \right|$$

Ab init spin-orbit pseudopotentials:

- Hartwigsen/Goedecker/Hutter pseudopotentials (*pspcod=3*)

→ $v_{NL}^{ion-so}=0$ and $v_{NL}^{so-ion}=0$

- Martins-Troullier pseudopotentials (*pspcod=5*)

$$V = V_L + \sum_{l,m} \begin{pmatrix} \left| v_l^{ion} Y_l^m \right\rangle & \left| v_l^{so} Y_l^m \right\rangle \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 \\ 0 & \frac{l(l+1)}{4} \end{pmatrix}_{Q_1} + (\vec{L} \cdot \vec{S}) \cdot \begin{pmatrix} 0 & 1 \\ 1 & -\frac{1}{2} \end{pmatrix}_{Q_2} \cdot \begin{pmatrix} \left| v_l^{ion} Y_l^m \right\rangle \\ \left| v_l^{so} Y_l^m \right\rangle \end{pmatrix}$$

→ Diagonalization of Q_2 ⇒ $v_{NL}^{ion-so}=0$ and $v_{NL}^{so-ion}=0$



Theoretical framework – Non-local operator implementation

$$\begin{aligned}
 V_{NL}(\vec{K}\sigma, \vec{K}'\sigma') &= \sum_{l,m} \left\langle \vec{K}\sigma \left| Y_{lm} u_l^{ion} \right\rangle E_{KB}^l \left\langle u_l^{ion} Y_{lm} \right| \vec{K}'\sigma' \right\rangle \quad v^{ion-ion} \\
 &\quad + \sum_{l,m} \left\langle \vec{K}\sigma \left| \vec{L} \cdot \vec{S} \right| Y_{lm} u_l^{ion} \right\rangle E_{KB}^l \left\langle u_l^{ion} Y_{lm} \right| \vec{L} \cdot \vec{S} \left| \vec{K}'\sigma' \right\rangle \quad v^{so-so} \\
 \sum_{l,m} \left\langle \vec{K}\sigma \left| Y_{lm} u_l^{ion} \right\rangle E_{KB}^l \left\langle u_l^{ion} Y_{lm} \right| \vec{K}'\sigma' \right\rangle &= 4\pi \cdot \sum_l (2l+1) \cdot E_{KB}^l \cdot f_l^{ion}(\vec{K}) \cdot f_i^{ion}(\vec{K}') \cdot P_l(\hat{K} \cdot \hat{K}') \cdot \delta_{\sigma\sigma'} \quad \text{1} \\
 \sum_{l,m} \left\langle \vec{K}\sigma \left| \vec{L} \cdot \vec{S} \right| Y_{lm} u_l^{ion} \right\rangle E_{KB}^l \left\langle u_l^{ion} Y_{lm} \right| \vec{L} \cdot \vec{S} \left| \vec{K}'\sigma' \right\rangle &= 4\pi \cdot \sum_l (2l+1) \cdot E_{KB}^l \cdot f_l^{SO}(\vec{K}) \cdot f_l^{SO}(\vec{K}') \\
 &\quad \times \left[\frac{P_l(\hat{K} \cdot \hat{K}') \cdot \frac{l(l+1)}{4} \delta_{\sigma\sigma'}}{\text{1,}} + P'_l(\hat{K} \cdot \hat{K}') \cdot \frac{i}{2} \cdot \frac{\vec{K} \times \vec{K}'}{\|\vec{K}\| \|\vec{K}'\|} \cdot \langle \sigma | \vec{S} | \sigma' \rangle \right] \quad \text{2}
 \end{aligned}$$

$$f_l^A(\vec{K}) = \int_0^\infty u_l^A(r) \cdot j_l(2\pi|\vec{K}|r) \cdot r^2 \cdot dr \quad \text{Form factor}$$

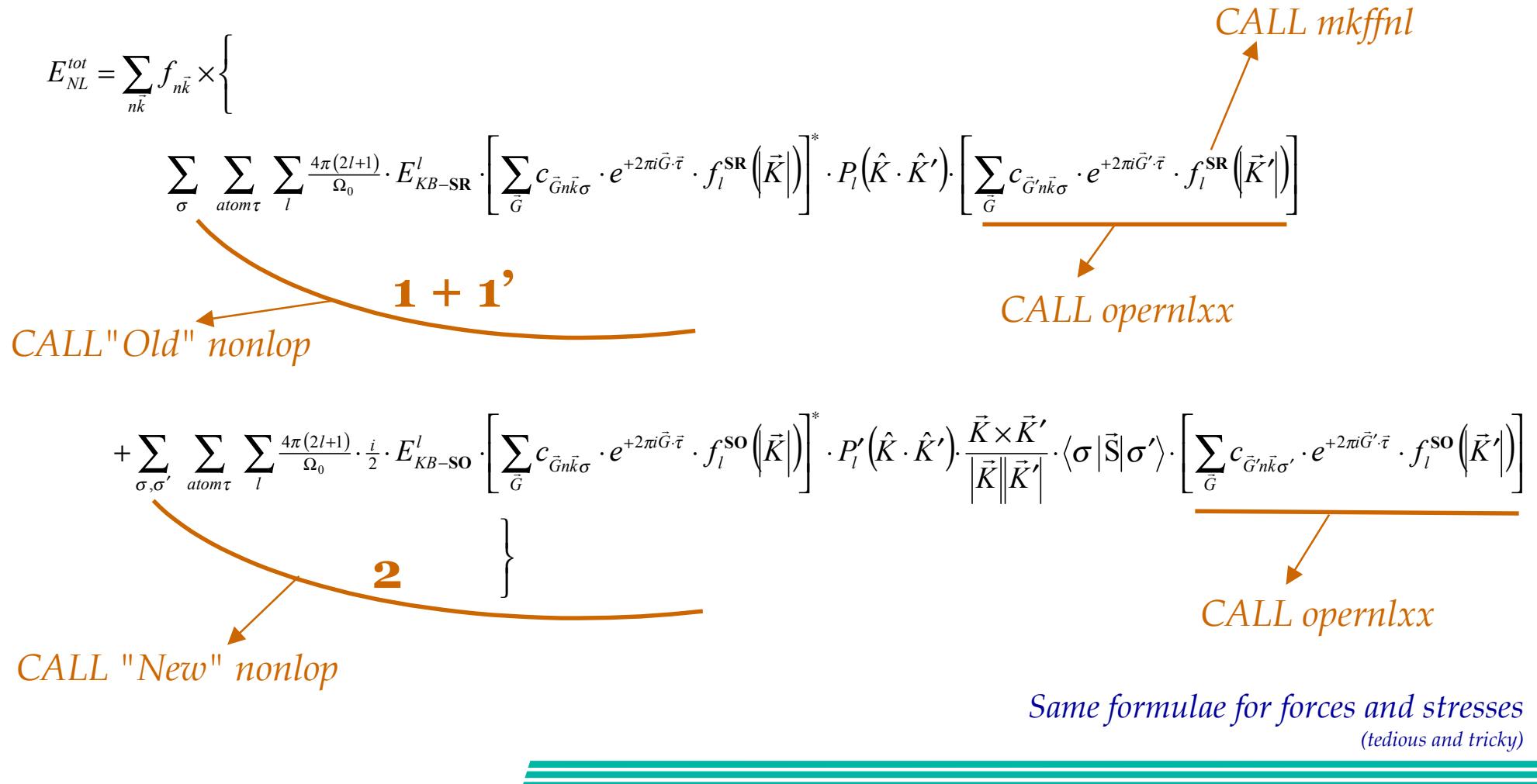
$$P_l(\hat{K} \cdot \hat{K}') = \frac{4\pi}{2l+1} \cdot \sum_m Y_{lm}(\hat{K}) \cdot Y_{lm}^*(\hat{K}') \quad \text{Legendre polynomial} \\ (\text{derivative: } P'_l)$$





Theoretical framework – Non-local operator implementation

$$E_{NL}^{tot} = \frac{1}{\Omega_0} \cdot \sum_{n\vec{k}} f_{n\vec{k}} \sum_{\vec{G}, \vec{G}'} \sum_{\sigma, \sigma'} \sum_{atom \tau} c_{\vec{G}n\vec{k}\sigma}^* \cdot e^{-2\pi i \vec{G} \cdot \vec{\tau}} \cdot V_{NL}(\vec{K}\sigma, \vec{K}'\sigma') \cdot e^{+2\pi i \vec{G}' \cdot \vec{\tau}} \cdot c_{\vec{G}'n\vec{k}\sigma'}$$



↳ Spin-orbit flag

$pspso \longrightarrow$ 1 = no spin-orbit interaction
2 = spin-orbit coupling

↳ Quantum numbers l, m, n, σ

$lmnmax \leftrightarrow lmnmmaxso$

$indlmn (1\dots 6, 1\dots lmnmmaxso, itype)$

l, m, n, ln, lm, σ

↳ Spinorial representation of wave-functions

$cg(2,\dots) \leftrightarrow cg(2,\dots \times nspinor)$

Nb of spinorial components

$\underbrace{cg(:,1)\dots\dots\dots\dots\dots\dots}_{\mathbf{cg}} \underbrace{cg(:,mcg)\dots\dots\dots\dots\dots\dots}_{\mathbf{cg}} \underbrace{cg(:,2 \cdot mcg)}_{\mathbf{cg}}$

↳ Non local form factors

 $ffnl(\dots, mpsang) \leftrightarrow ffnl(\dots, mpssolang)$

$$\underbrace{ffnl(\dots, 1)}_{\mathbf{ffnl} - \mathbf{s}} \dots \underbrace{ffnl(\dots, 2)}_{\mathbf{ffnl}^{\text{SR}} - \mathbf{p}, \mathbf{d}, \mathbf{f}} \dots \dots \dots \underbrace{ffnl(:, mpsang)}_{\mathbf{ffnl}^{\text{SO}} - \mathbf{p}, \mathbf{d}, \mathbf{f}} \dots \dots \dots \underbrace{ffnl(:, mpssolang)}_{\mathbf{ffnl}^{\text{SO}} - \mathbf{p}, \mathbf{d}, \mathbf{f}}$$

↳ KB energies

 $ekb(\dots, lnmax) \leftrightarrow ekb(\dots, lnmaxso)$

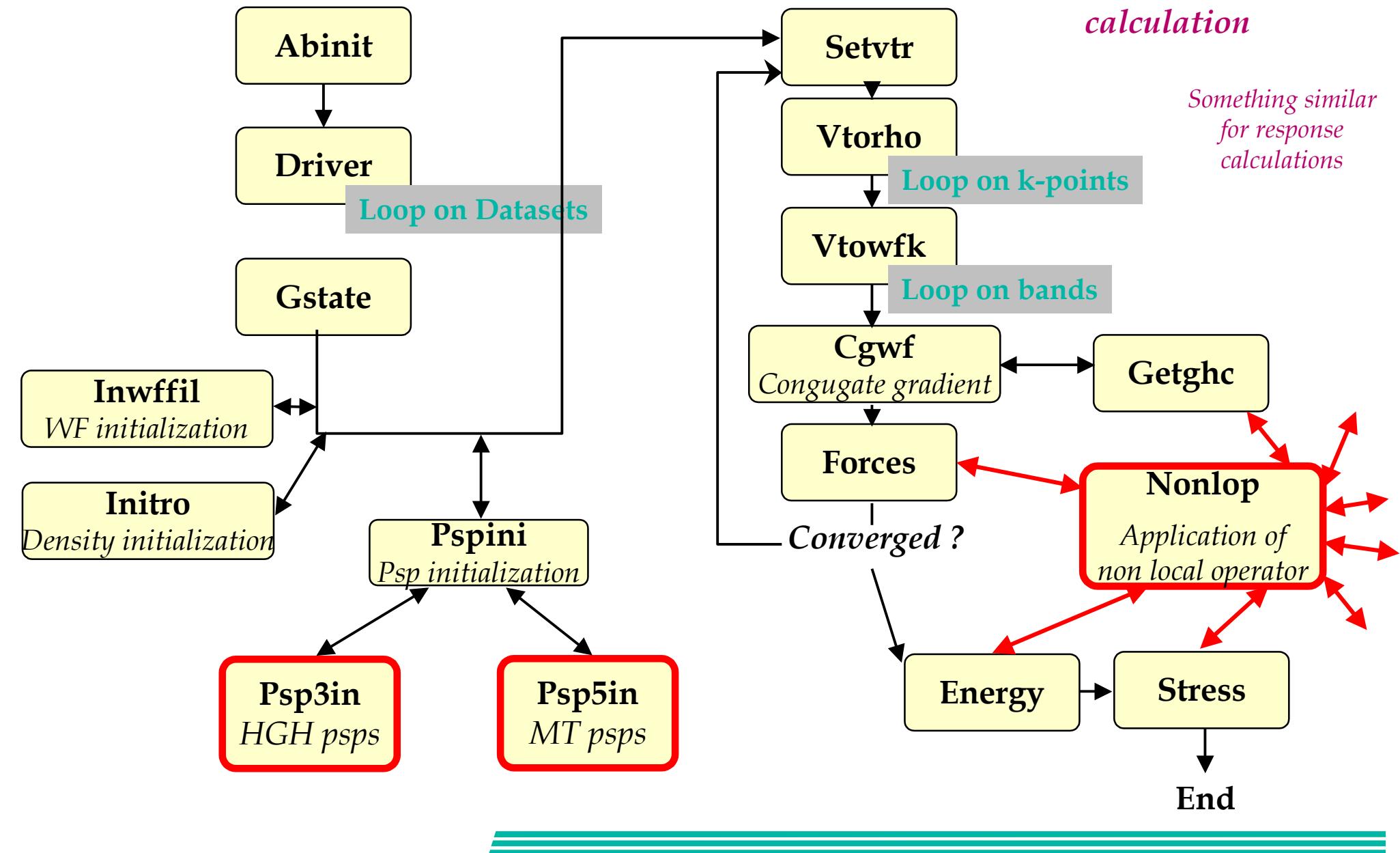
$$\underbrace{ekb(\dots, 1)}_{\mathbf{ekb} - \mathbf{s}} \dots \underbrace{ekb(\dots, 2)}_{\mathbf{ekb}^{\text{SR}} - \mathbf{p}, \mathbf{d}, \mathbf{f}} \dots \dots \dots \underbrace{ekb(:, lnmax)}_{\mathbf{ekb}^{\text{SO}} - \mathbf{p}, \mathbf{d}, \mathbf{f}} \dots \dots \dots \underbrace{ekb(:, lnmaxso)}_{\mathbf{ekb}^{\text{SO}} - \mathbf{p}, \mathbf{d}, \mathbf{f}}$$



Abinit v3 modifications – Routines

Ground state calculation

Something similar
for response
calculations





Focus on...



Psp5in.f

Martins-Trouiller pseudopotentials initialization

- ✓ Read psp info in MT format
- ✓ Diagonalize Q_2 matrix in order to cancel v^{ion-so} and v^{so-ion}
- ✓ Mix v^{ion} and v^{so} into v^{SR} and v^{SO}
- ✓ Initialize corresponding E_{KB} and form factors

Trick : uses 2 projectors,
one for v^{ion} , one for v^{SO}



Focus on...



nonlop.f Application of non local operator

Compute quantities like $V_{NL}|\vec{n}\vec{k}\sigma\rangle$, $\sum_{n\vec{k}\sigma} f_{n\vec{k}} \cdot \langle n\vec{k}\sigma | V_{NL} | n\vec{k}\sigma \rangle$, $\frac{\partial}{\partial \dots} \sum_{n\vec{k}\sigma} f_{n\vec{k}} \cdot \langle n\vec{k}\sigma | V_{NL} | n\vec{k}\sigma \rangle$

- ✓ Compute $\left[\sum_{\vec{G}} c_{\vec{G}'n\vec{k}\sigma} \cdot e^{+2\pi i \vec{G}' \cdot \vec{r}} \cdot f_l^X(|\vec{K}'|) \right]$ for SR and SO
(call to opernl)
- ✓ Loop on spins, atoms and angular momenta
- ✓ Compute application of $V^{SR\uparrow}$, $V^{SR\downarrow}$ and V^{SO}
[see **(1+1') \uparrow** , **(1+1') \downarrow** and **2 $\uparrow\downarrow$**]
- ✓ Terms like $f_l^X(|\vec{K}|) \cdot f_l^X(|\vec{K}'|) \cdot P_l(\hat{K} \cdot \hat{K}')$ are developed on cubic harmonics



Running Abinit with spin-orbit coupling – Pseudopotential files

Hartwigsen, Goedecker, Hutter pseudopotentials

pspcod=3

Nothing to change !

Usual header for Abinit's psp's

Hartwigsen-Goedecker-Hutter psp for Ta, from PRB58, 3641 (1998)									
73	13	992211	zatom,zion,pspdat						
3	2	2	0	2001	0	pspcod,pspxs,lmax,lloc,mmax,r2well			
0.550000	4.546236	0.779422	0		0	rloc, c1, c2, c3, c4			
0.421853	2.708136	-5.790959	0.947663			rs, h11s, h22s, h33s			
0.461345	-0.724853	-2.215211	0			rp, h11p, h22p, h33p			
	0.649992	-0.336371	-0.101322				k11p, k22p, k33p		
0.410994	1.348495	-5.386947	0			rd, h11d, h22d, h33d			
	0.205344	-0.102353	0				k11d, k22d, k33d		

Directly from HGH table

Spin-orbit terms

||||| Running Abinit with spin-orbit coupling – Pseudopotential files

This file contains information about the use of spin-orbit
for format pspcod=5 of pseudopotentials.
Copyright (C) 2000-2002 ABINIT group (FJ,XG)
This file is distributed under the terms of the GNU General Public License, see
~ABINIT/Infos/copyright or <http://www.gnu.org/copyleft/gpl.txt> .
For the initials of contributors, see ~ABINIT/Infos/contributors.

- 1) The line containing Haman grid parameters must be completed by an information about the spin-orbit format of the psp.

So, one replaces

```
2.508991628593723E-4  0.0125          r1,al  
by  
2.508991628593723E-4  0.0125  2      r1,al,pspso
```

pspso is 1 for non spin-orbit (optional), 2 for spin-orbit

- 2) The lines describing the number of projectors and some of their characteristics must be duplicated, as soon as l/=0.

The number of projectors must be 2.

So, one replaces

```
0   0   0   1   2.76      1,e99.0,e99.9,nproj,rcpsp  
.000   .00000   .00000   .000   rms,ekb1,ekb2,epsatm  
1   0   0   1   3.91      1,e99.0,e99.9,nproj,rcpsp  
.000   .00000   .00000   .000   rms,ekb1,ekb2,epsatm  
2   0   0   1   1.57      1,e99.0,e99.9,nproj,rcpsp  
.000   .00000   .00000   .000   rms,ekb1,ekb2,epsatm
```

by

```
0   0   0   1   2.76      1,e99.0,e99.9,nproj,rcpsp  
.000   .000   .000   .000   rms,ekb1,ekb2,epsatm  
1   0   0   2   3.91      1,e99.0,e99.9,nproj,rcpsp  
.000   .000   .000   .000   rms,ekb1,ekb2,epsatm  
1   0   0   2   3.91      1,e99.0,e99.9,nproj,rcpsp  
.000   .000   .000   .000   rms,ekb1,ekb2,epsatm  
2   0   0   2   1.57      1,e99.0,e99.9,nproj,rcpsp  
.000   .000   .000   .000   rms,ekb1,ekb2,epsatm  
2   0   0   2   1.57      1,e99.0,e99.9,nproj,rcpsp  
.000   .000   .000   .000   rms,ekb1,ekb2,epsatm
```

- 3) The pseudopotentials and pseudowavefunctions are then entered, in the order s, p1/2, p3/2, d3/2, d5/2, f5/2, f7/2.

Martins-Troullier
pseudopotentials

pspcod=5

Infos/Psp_infos/
psp5spinorbit.info
file

V 3.4 format !



Running Abinit with spin-orbit coupling – Pseudopotential files

Martins-Troullier pseudopotentials $pspcod=5$

```
Uranium LDA-SO, Martins-Trouiller, spdf, S local part
92.00000 14.00000 990913 zatom, zion, pspdat
5 2 3 0 1063 .00 pspcod,pspxc,lmax,1loc,mmax,r2well
1.99083031399284E-4 0.0125 2 r1,al,psps00
0 0 0 1 1.3 1,e99.0,e99.9,nproj,rcpssp s
.000 .000 .000 .000 rms,ekb1,ekb2,epsatm
1 0 0 2 1.7 1,e99.0,e99.9,nproj,rcpssp p3/2
.000 .000 .000 .000 rms,ekb1,ekb2,epsatm
1 0 0 2 1.7 1,e99.0,e99.9,nproj,rcpssp p1/2
.000 .000 .000 .000 rms,ekb1,ekb2,epsatm
2 0 0 2 2.20 1,e99.0,e99.9,nproj,rcpssp d5/2
.000 .000 .000 .000 rms,ekb1,ekb2,epsatm
2 0 0 2 2.20 1,e99.0,e99.9,nproj,rcpssp d3/2
.000 .000 .000 .000 rms,ekb1,ekb2,epsatm
3 0 0 2 1.3 1,e99.0,e99.9,nproj,rcpssp f7/2
.000 .000 .000 .000 rms,ekb1,ekb2,epsatm
3 0 0 2 1.3 1,e99.0,e99.9,nproj,rcpssp f5/2
.000 .000 .000 .000 rchrg,fchrg,qchrg
0 0 0
0 =1 for pseudopotential
[...]
1 =1 for pseudopotential
[...]
1 =1 for pseudopotential
[...]
0 =1 for wavefunction
[...]
```

Usual header

1 for non-SO (optional)
2 for SO

nproj must be 2,
except for l=0

The pseudopotentials
and
pseudowavefunctions
are entered, in the
order s, p1/2, p3/2,
d3/2, d5/2, f5/2,
f7/2.

lloc=0 refers to the s potential
lloc=1 refers to the p3/2 potential
lloc=2 refers to the d5/2 potential
lloc=3 refers to the f7/2 potential
lloc=-1 refers to the p1/2 potential
lloc=-2 refers to the d3/2 potential
lloc=-3 refers to the f5/2 potential

V 3.4 format !

Abinit.help – Input variables**nspinor**

Mnemonics: Number of SPINORial components of the w-functions

Characteristic: DEVELOP

Variable type: integer parameter

The Default is 1.

If nspinor=1, usual case : scalar wavefunction (compatible with (nsppol=1, nsden=1) as well as (nsppol=2, nsden=2))

If nspinor=2, the wavefunction is a spinor (compatible with nsppol=1, with nsden=1 or 4, but not with nsppol=2)

When nspinor is 2, the values of istwfk are automatically set to 1. Also, the number of bands, for each k-point, should be even.



Abinit.help – Input variables

pspso

Mnemonics: PSeudoPotential: treatment of Spin-Orbit interaction

so_typat

Mnemonics: Spin-Orbit: TYPe of each pseudo-Atom

(alias to *pspso*, for the time being)

Variable type: integer array pspso(ntype)

The Default is ntype*1

For each type of atom (each psp), specify the spin-orbit interaction

If 1 : no spin-orbit interaction, even if nspinor=2

If 2 : treat spin-orbit in the HGH form (not allowed for all psp's)

If 3 : treat spin-orbit in the HFN form (not allowed for all psp's)

Also, pspso=0 default to 1, 2, or 3 according to the data contained in the pseudopotential file (1= there is no spin-orbit information in the psp file; 2= the spin-orbit information is of the HGH form; 3= the spin-orbit information is of the HFN form)

||||| Running Abinit with spin-orbit coupling – Input file

```
# -----  
# -           Input file for Abinit      -  
# -           U Alpha                   -  
# -----  
  
# 1-Options for output:  
# -----  
  prtwf 0  prtdos 0  enunit 2  
  
# 2-Parameters governing the convergence:  
# -----  
  ecut 90.  ecutsm 0.5  
  nband 38  nline 5  ntime 25  nstep 30  
  toldfe 1.d-10  tolmx 2.5d-5  strfact 25.  
  
# 3-Options for the choice of calculation:  
# -----  
  ixc 2  occopt 7  tsmear 0.01  
  optcell 3  ionmov 2  
  nspinor 2  pspso 2
```

Use 2 spinorial components

Use spin-orbit part of psp

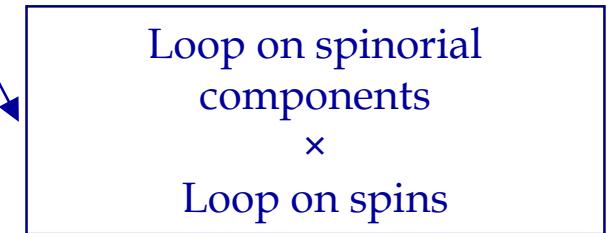
```
# 4-Definition of the unit cell:  
# -----  
  acell 3*5.2131723  
  rprim  0.5 -0.96748678  0.  
          0.5  0.96748678  0.  
          0.   0.           1.7682284  
  xred   1.07E-01 -1.07E-01 -2.5E-01  
          -1.07E-01  1.07E-01  2.5E-01  
  natom  2  ntype 1  type 2*1  
  zatnum 92.  amu 238.029  
  nsym  0  
  
# 5-Definition of special K-points:  
# -----  
  nkpt 0  kptopt 1  ngkpt 11 11 11  
  nshiftk 1  shiftk 0. 0. 0.
```



Running Abinit with spin-orbit coupling – Outline

You'll have to...

1. Build SO pseudopotential file
or read it from Abinit's compilation.
2. Set variables $nspinor$ and $pspso$ to the correct values in Abinit's input file.
3. Submit the job and wait... It takes 3/4 times more time than non-SO jobs.



||||| *Testing the spin-orbit coupling in Abinit*

Tantalum - Spin-orbit correction

	FPLMTO (Ha)	Abinit HGH (Ha)	Abinit MT (Ha)
$\Delta 5d$	0,0218	0,02134	0,02049
$\Delta 6p$	0,0193	0,01882	0,01857



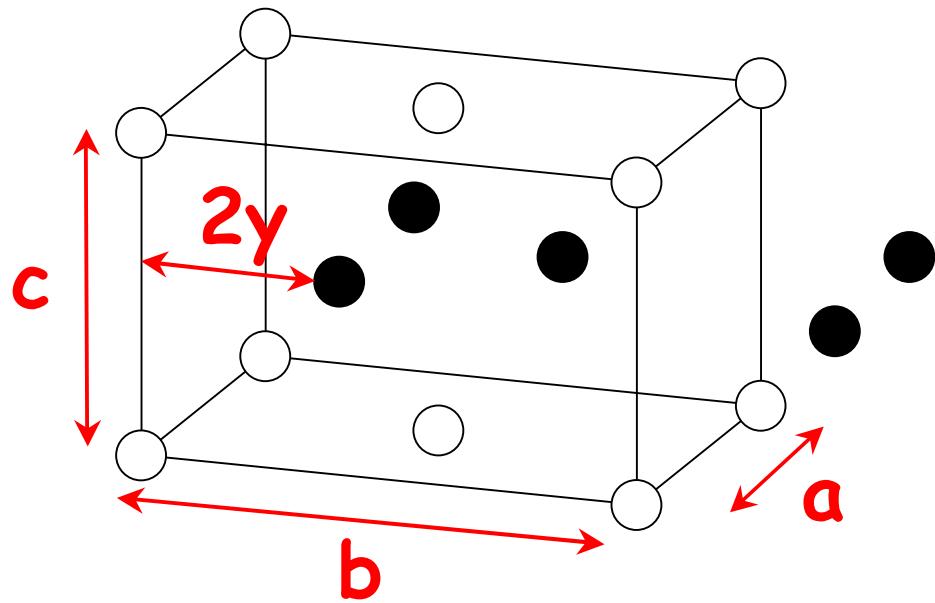
An example : α -uranium

- Actinides : Influence of spin-orbit coupling cannot be neglected
- Light actinides behave like 5d metals ;
f-electrons are delocalized.
- Uranium : third actinide $Z=92$ [Rn]6d¹5f³7s²
 α -phase stable at low temperature and pressure
- α structure : 4 structural parameters
Full relaxation is available with Abinit
- State of the art :
 - *Experimental data* available
 - *FLAPW, FPLMTO results*
Without FULL relaxation





α -uranium



Experimental data [1]

$a=0,2858 \text{ nm}$
 $a=2,0$
 $a=1, 3$
 $=0,105 \text{ nm}$
 $_{\text{o}}=138,9 \text{ u.a.}$
 $_{\text{o}}=135,5 \text{ GPa}$

[1] J. Akella, S. Weir, J.M.Wills, P. Soderlind,
J. Phys. : Condens. Matter 9, L549-L555 (1997)





Uranium : pseudopotentials

$6s^2 7s^0 6p^6 6d^1 5f^3 6d^1$

r_c	u.a.
6s	1,28
6p	1,52
6d	2,21
5f	1,28

LDA (erde n er, 1 81

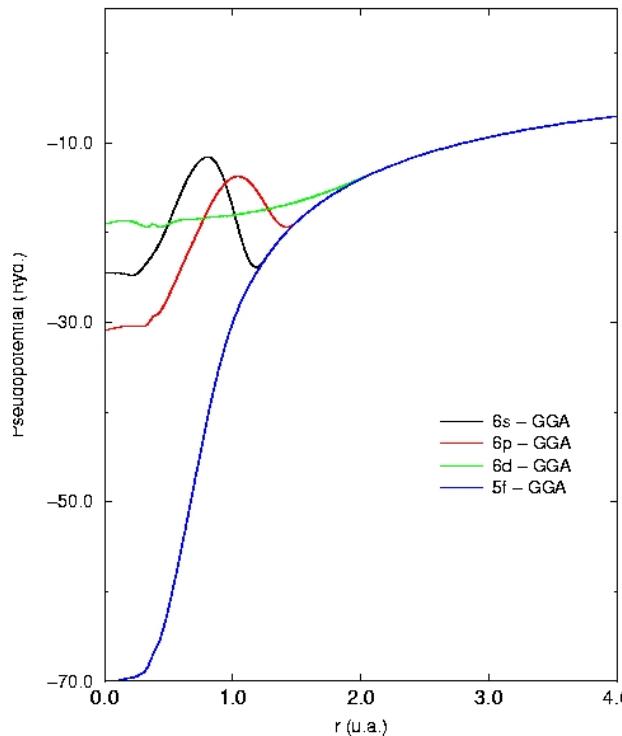
LDA + sp n r

GGA (erde r e rn er f, 1 6

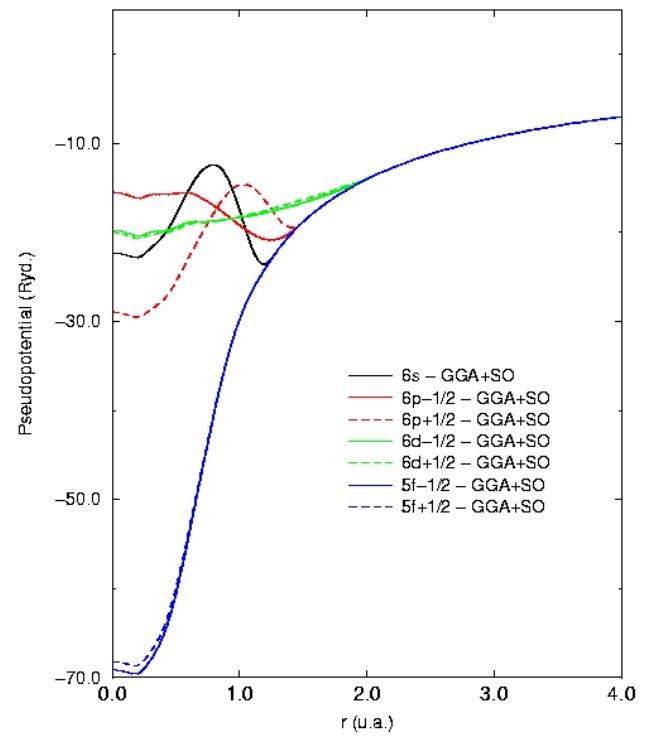
GGA + sp n r

Local part s

Pseudopotential for uranium – GGA approximation



Pseudopotential for uranium – GGA+Sin-orbit appproximation



Total energy converged with

Ecut=140 Ryd. , 64 k pts

Structural parameters converged with

Ecut=180 Ryd. , 216 k pts

Uranium : input file

```
#-----  
# - Input file for Abinit -  
# - U Alpha -  
#-----  
  
ndtset 7 igurewf 0 getxred 0  
acell1 3*5.15 acell2 3*5.20  
acell3 3*5.25 acell4 3*5.30  
acell5 3*5.35 acell6 3*5.40  
acell7 3*5.45  
  
# 1-Options for output:  
#-----  
prtwf 0 prtdos 0 enunit 2  
  
# 2-Parameters governing the convergence:  
#-----  
ecut 90. ecutsm 0.5  
nband 38 nline 5 ntime 25 nstep 30  
toldfe 1.d-10 tolmxm 2.5d-5 strfact 25.  
  
# 3-Options for the choice of calculation:  
#-----  
ixc 11 occopt 7 tsmeir 0.01  
optcell 3 ionmov 2  
nspinor 2 pspso 2
```

Several volumes

Ecut=180 Ryd.

216 k points

```
# 4-Definition of the unit cell:  
#-----  
acell 3*5.2131723  
rprim 0.5 -0.96748678 0.  
0.5 0.96748678 0.  
0. 0. 1.7682284  
xred 1.07E-01 -1.07E-01 2.5E-01  
-1.07E-01 1.07E-01 2.5E-01  
natom 2 ntype 1 type 2*1  
zatnum 92. amu 238.029  
nsym 0  
  
# 5-Definition of special K-points:  
#-----  
nkpt 0 kptopt 1 ngkpt 11 11 11  
nshiftk 1 shiftk 0. 0. 0.
```

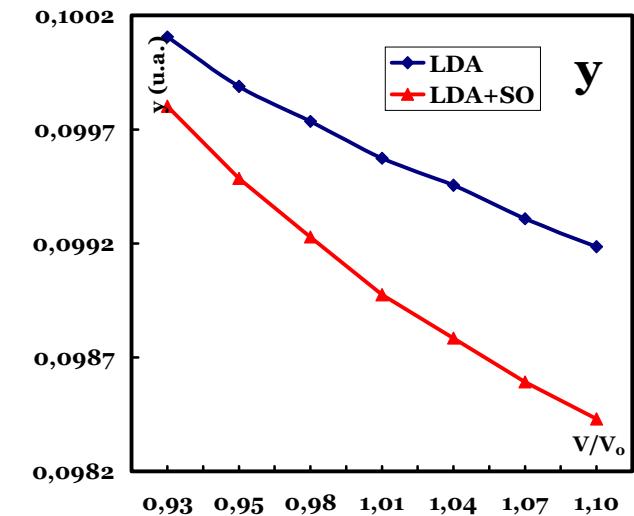
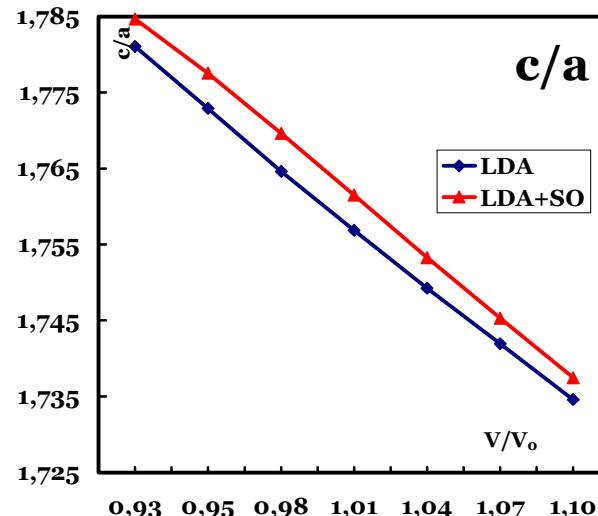
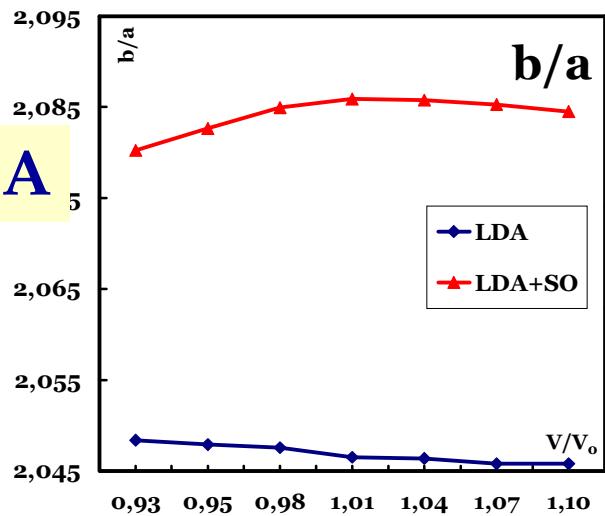
GGA

Spin-orbit

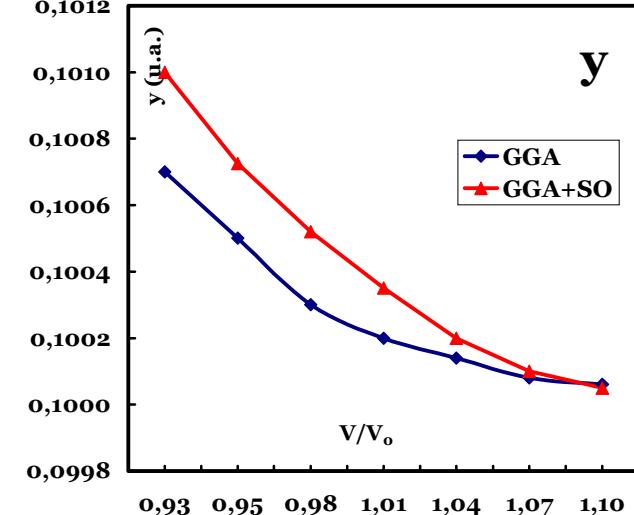
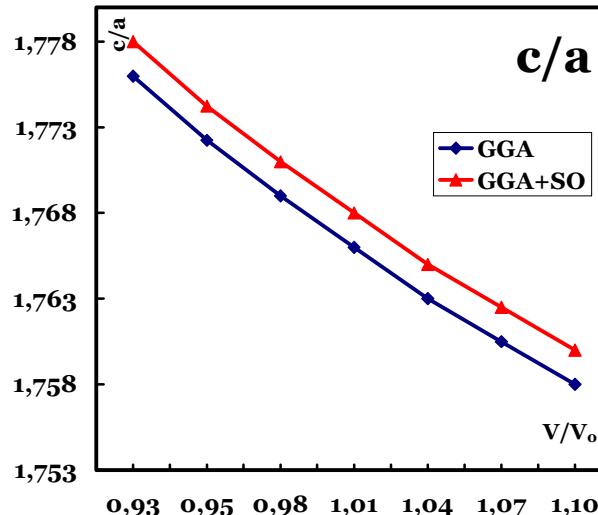
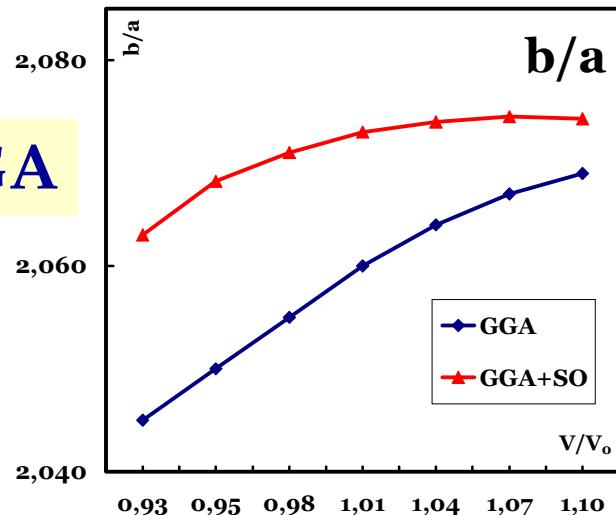
FULL relaxation
at constant volume

Uranium : structural parameters

LDA



GGA





Uranium : Volume and bulk modulus

Equilibrium volume V_o (u.a.)

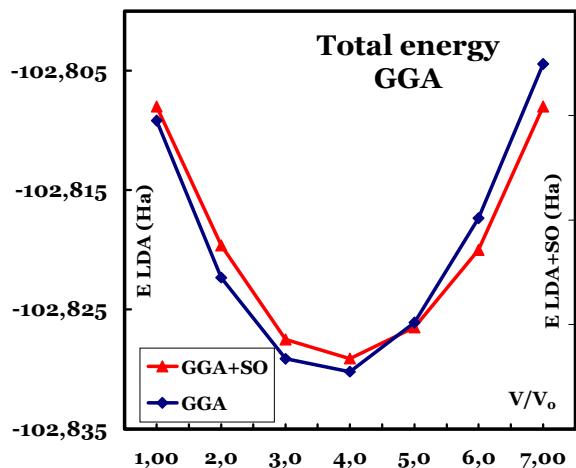
	ABINIT				FLAPW - Jones et al[1]				FPLMTO - Soderlind[2]		Exp.
	LDA	LDA+	GGA	GGA+	LDA	LDA+	GGA	GGA+	LDA+	GGA+	
Without relaxation	133,6	135,2	137,2	1 5,6	127,	128,5	137,7	1 0,1	123,7	131,5	138,
With relaxation	126,6	13 ,	13 ,5	13 ,6							138,

Bulk modulus B (GPa)

	ABINIT				FLAPW - Jones et al[1]				FPLMTO - Soderlind[2]		Exp.
	LDA	LDA+	GGA	GGA+	LDA	LDA+	GGA	GGA+	LDA+	GGA+	
Without relaxation	181	160	1 1	126	176	1	1	12	2 0	172	135
With relaxation	173	16	1 6	128							135

[1] M.D. Jones, J.C. Boettger, R.C. Alberts et D.J. Singh. Phys. Rev. B, **61**, 4644 (2000)

[2] P. Soderlind, O. Eriksson, B. Johansson et J.M. Wills, Phys. Rev. B **50**, 7291 (1994)



► GGA approximation
pin or it co plin

Increase e
Decrease

r d s e

Best result with
GGA
+ Spin-orbite
+ full relaxation



To be continued...

Spin-orbit implemented for
Energy
Forces
Stresses
Response to atomic displacements

To be implemented for response to electric field

Completely tested
Comparison with FPLMTO
Consistency : forces, stresses, phonons
and derivatives of the energy...
Physics : Ta, Ce, U, ...

See Test_v3

PAW + SO ??? Soon ?

Difficulty :

- Legendre polynomials representation of V_{NL} not usable anymore
- *Nonlop* subroutine completely new
- Formulae and tricks used to program spin-orbit coupling with Legendre polynomials not valid anymore